Assessment Plan for Benzene, C_{6-12} Alkyl Derivatives (CAS#68608-80-0, Alkylate Top) in Accordance with the USEPA High Production Volume Challenge Program

Prepared for

Huntsman LLC

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I. INTRODUCTION

The High Production Volume (HPV) Challenge Program is a voluntary initiative of the US chemical industry to complete hazard data profiles for approximately 2800 HPV chemicals as identified on the US Environmental Protection Agency's (USEPA) 1990 Toxic Substances Control Act (TSCA) Inventory Update Rule (IUR). In the US, HPV chemicals are those that are manufactured or imported in quantities greater than 1 million pounds per year. The hazard data to be provided in the program are those that meet the requirements of the Screening Information Data Set (SIDS) Program. SIDS, which has been internationally agreed to by member countries of the Organization for Economic Cooperation and Development (OECD), provides the basic screening data needed for an initial assessment of the physical-chemical properties, environmental fate, and adverse human and environmental effects of chemicals. The information for completing the SIDS can come from existing data or may be generated as part of the HPV Challenge Program. Once the available studies are identified or conducted, "robust summaries" are prepared. These summaries are then entered into the standard International Uniform Chemical Information Database (IUCLID) software and present the salient information from each of the reliable studies.

The USEPA, industry, and non-governmental organizations (NGOs) are unified in their commitment to minimize the numbers of animals tested in the HPV Challenge Program whenever it is scientifically justifiable. One approach toward this consideration is to evaluate closely related chemicals as a group, or category, rather than solely as individual chemicals. This approach takes advantage of structure activity relationships (SARs), which is based on the understanding that chemicals with similar structures often have similar and/or predictable characteristics and behavior in the environment and in mammalian systems. The use of categories and SARs is encouraged by USEPA in the HPV Challenge Program. Appropriate use of SARs can allow for a more efficient evaluation of the available data and significantly reduce the number of animals required for testing.

Huntsman LLC (formerly Huntsman Corporation) has agreed to assemble and review available public and private toxicological data, develop and provide an assessment plan for the sponsored material and conduct additional research, including testing when necessary, for a mixture of alkylated benzenes and *n*-paraffins (CAS #68608-80-0; hereafter referred to as an "Alkylate Top"). While Huntsman LLC is not proposing this material as part of a category approach *per se*, as a mixture it is appropriate to review the pertinent data of the principal constituents using SAR as a means to help characterize the Alkylate Top's properties and characteristics.

This assessment plan is the result of Huntsman LLC's efforts and provides a summary and analysis of the available data, and identifies any data gaps in the SIDS data profile. Section II of this assessment plan provides a characterization of the sponsored Alkylate Top production process and use patterns. Section III reviews the methods used in the collection of published and unpublished data. Section IV reviews the evaluation of data quality. Section V is an in-depth evaluation of the available data, first for the Alkylate Top itself, then for its principal constituents and for Linear Alkylbenzene (LAB). Section VI is a summary of the Alkylate Top and constituents properties. Section VII presents the conclusions regarding data availability.

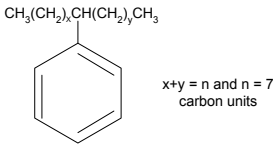
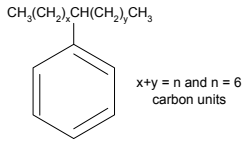
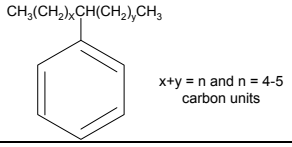
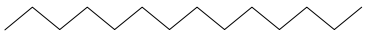
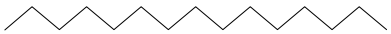
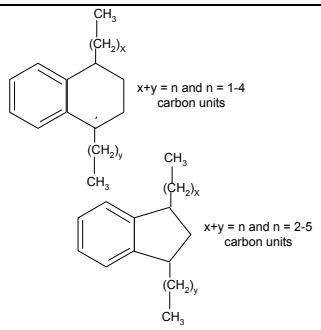
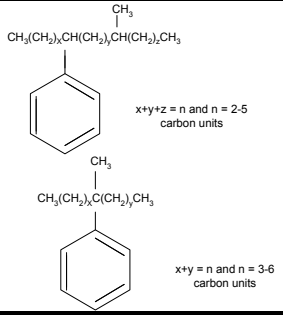
II. IDENTIFICATION OF THE SPONSORED MIXTURE

A. Production Process

Huntsman LLC is sponsoring Benzene, C_{6-12} alkyl derivatives (CAS #68608-80-0; called "Alkylate Top" hereafter), in the USEPA HPV Challenge Program. This Alkylate Top is a mixture of aromatic and aliphatic hydrocarbons derived as a low boiling point co-product from the LAB manufacturing process. The LAB production process entails the partial conversion of C_{10-14} *n*-paraffins to internal *n*-olefins by catalytic dehydrogenation. The resulting mixture of *n*-paraffins and *n*-olefins is selectively hydrogenated to reduce diolefins and fed into an alkylation reactor together with benzene (in excess) and hydrofluoric acid as a catalyst for the Friedel-Crafts reaction producing C_{10-14} secondary linear alkylbenzenes (LAB). The Alkylate Top results from an intermediate distillation cut prior to the isolation of the final LAB product and serves to remove impurities with a lower boiling point than LAB. Following the removal of the Alkylate Top, a final distillation removes commercial detergent grade LAB as the distillate.

This production process results in an alkylated benzene mixture, the Alkylate Top, which consists predominantly of C_{7-10} secondary linear alkylbenzenes, C_{14} paraffin, other aromatics (mainly dialkylindanes and dialkyltetralins), and other LAB (likely mono-methyl branched [iso-LAB]). Overall, the Alkylate Top consists of approximately 48-56% C_7-C_{10} linear alkylbenzenes, 13-35% paraffins, 8% dialkylindanes/tetralins, and 6-22% iso-LAB. The current Alkylate Top product is designated L210 by Huntsman LLC. Fractions of L210 may vary slightly depending on whether the samples are collected during light (L210L) or heavy (L210H) fractionation, which differ slightly due to slight differences in the chain length distribution of the paraffin employed during LAB production. Table 1 shows representative structures of the constituents that make up greater than 99% of the current Alkylate Top mixture based on chemical analyses conducted in the fall of 2002 (Rapko 2002). The ranges for light and heavy paraffin samples are shown separately, although in practice the two are not segregated and only the combined L210 product is distributed.

Table 1. Representative Structures of the Constituent Compounds of the Alkylate Top

COMPOUND	Relative % - Light [Mean]	Relative % - Heavy [Mean]	REPRESENTATIVE STRUCTURE
C_{10}-LAB	15-34 [23]	25-36 [30]	
Sec-nonylbenzene	14-34 [24]	2-9 [8]	
Sec-octylbenzene/ heptabenzene	7-11 [9]	8-11 [10]	
n-Tetradecane	4-20 [13]	31-39 [35]	
n-Pentadecane	0.3-0.4 [0.3]	0.3-0.7 [0.5]	
Other Components (mainly dialkylindanes and dialkyltetralins)	5-12 [8]	8-9 [8]	
Other LAB (likely mono-methyl branched [iso-LAB])	20-27 [22]	5-8 [6]	

Note: Relative percent shows the range of 10 samples during light (L) and 11 samples during heavy (H) paraffin campaigns collected from September-October 2002 at the Chocolate Bayou, Texas, LAB production unit. Samples were analyzed by GC and GC/MS.

B. Relationship to Tested Materials

The current Alkylate Top material is approximately 48-56% C_7-C_{10} linear alkylbenzenes, 13-36% paraffins, 8% other components from the dehydrogenation process (mainly dialkylindanes and dialkyltetralins), and 6-22% iso-LAB. The Alkylate Top material used in much of the biodegradation and toxicity testing consisted of approximately 44% alkylbenzenes, 29% paraffins, and 24% dialkylindanes.

Furthermore, in the earlier production of Alkylate Tops, the two fractions (L210L and L210H) were used separately and therefore underwent separate safety and toxicity testing. Due to modifications in the efficiency of the production process, the L210L and L210H fractions are no longer segregated and are considered a single mixture designated as L210. The modification in the production process also has significantly reduced the occurrence of dialkylindanes and dialkyltetralins. For example, in a biodegradation study conducted on a Monsanto Alkylate Top mixture in 1980, the test material included a substantial amount of alkylindanes (24%). Chemical analysis of the current Alkylate Top (Rapko 2002) resulted in a substantially lower amount, with 7-9% other components of the dehydrogenation process considered to be mainly dialkylindanes and dialkyltetralins. Dialkylindanes and dialkyltetralins, and other LAB (likely mono-methyl branched [iso-LAB]), are known to be formed in the LAB production process (de Almeida et al. 1994; Nielsen et al. 1997). Concentrations in LAB range from <1% to 8% dialkylindanes and dialkytetralins and <1% to 6% iso-LAB.

The alkylbenzene constituents of the Alkylate Top are secondary linear or mono-methyl branched alkyl chain materials (e.g., C_{7-9} linear alkylbenzenes, C_{10}-LAB, and iso-LABs) that can be attached to the benzene ring at the 2, 3, 4, or 5 positions. However, the primary alkylbenzenes (e.g., nonyl- and decylbenzene) are chemical isomers and would be expected to have properties essentially similar to the secondary alkylbenzenes. Therefore, data for the primary alkylbenzenes are utilized where appropriate. Similarly, data for the C_{14} and C_{15} paraffin constituents of the Alkylate Top are included when available[1]. Because the Alkylate Top is derived as a co-product from the LAB manufacturing process, and because LAB has been extensively studied, LAB data are provided as a benchmark for comparison.

C. Use Patterns and Exposure Potential

Currently, 100% of the sponsored Alkylate Top is sold into the marine diesel fuel market as a blend stock for viscosity control. This is the only commercial use of the material. During production, it is sufficient for workers to employ standard personal protective equipment to minimize exposure. During use, very limited human and environmental exposure to marine diesel fuel is expected, given its destruction during the combustion process. Environmental exposure may occur if the diesel fuel is spilled in transit and thus presents the same limited exposure potential as other types of fuel spills. Because the Alkylate Top is only a component of the fuel, the potential for significant exposure would be even further reduced.

[1] Additional data relevant to the evaluation of the constituent paraffin materials are being compiled by the American Chemistry Council Hydrocarbon Solvents Panel.

III. COLLECTION OF PUBLISHED AND UNPUBLISHED DATA

Huntsman LLC contributed in-house data on physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity for the sponsored Alkylate Top mixture. To supplement these data, literature searches were conducted of on-line databases (e.g., Hazardous Substances Databank [HSDB], Registry of Toxic Effects of Chemical Substances [RTECS], and Aquatic Toxicity Information Retrieval [AQUIRE]), standard scientific data compendia (e.g., *CRC Handbook of Chemistry and Physics* and *The Merck Index*), and other published sources (e.g., International Uniform Chemical Information Database [IUCLID]). The literature search encompassed the Alkylate Top itself, as well as its principal constituents and the structural similar primary linear alkylbenzenes. Chemical analysis of the Alkylate Top was conducted in the fall of 2002 to characterize its constituent makeup (Rapko 2002). All of these sources were used to compile the data presented in this document.

IV. EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY

The collected data were reviewed for quality and acceptability following the general USEPA and OECD SIDS guidance and the systematic approach described by Klimisch et al. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. The Klimisch approach specifies four categories of reliability for describing data adequacy. These are:

1 **Reliable without Restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

2 **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

3 **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

4 **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g., listed in abstracts or secondary literature.

Only those studies which are deemed reliable for current HPV Challenge Program purposes are included in the data set for this assessment plan. Reliable studies include both categories rated 1 (Reliable without restriction) and 2 (Reliable with restrictions). Studies rated 3 (Not reliable) were not used. Studies rated 4 (Not assignable) were used when professional judgment deemed it appropriate as part of a weight-of-evidence approach. Finally, some older studies were not included if they had been superceded by more recent studies rated 1.

Some of the available data were from study reports conducted by either outside contract laboratories or in-house industry laboratories. These study reports followed standard procedures for testing of physical-chemical properties, environmental fate and transport, aquatic toxicity, and mammalian toxicity. The most recent studies were conducted under GLP provisions. Additional data were obtained from the published, peer-reviewed, scientific literature. Reliable data from all of these sources were incorporated into the data set as appropriate.

V. EVALUATION OF THE AVAILABLE DATA

All of the available data were compiled and robust summaries were prepared according to the format recommended by the USEPA and OECD. These summaries were then entered into the standard International Uniform Chemical Information Database (IUCLID) software and present the salient information from each of the reliable studies. All of the summaries are collected into a dossier that includes the sponsored Alkylate Top mixture as well as its principal constituents and structurally related materials. In addition, because the Alkylate Top is formed during the production process for LAB and its constituents include structural similarities, data for LAB are included. The dossier containing the robust summaries for the Alkylate Top and related chemicals should be used in conjunction with this assessment plan.

Table A-1 in the Appendix to this assessment plan is a matrix of SIDS/HPV endpoints and the available data for the sponsored Alkylate Top and related materials. The table includes data for LAB as a benchmark for comparison. The materials are organized left to right in the table beginning with LAB, followed by the sponsored Alkylate Top, the principal constituents of the Alkylate Top mixture (pentadecane, tetradecane, and C_{10}-LAB), and then the structurally similar primary C_9 and C_{10} linear alkylbenzenes. Data drawn from the robust summaries are shown in the table for each endpoint when available. Endpoints for which specific data are not available are identified by "--" in the table. The data presented for LAB were obtained from a completed European dossier and risk assessment report (Revision June 1997) and an updated USEPA SIDS report provided to OECD in 2002. The extent to which each of the endpoints is adequately characterized by the available data is evaluated.

A. *Evaluation of the Available Data on the Alkylate Top*

Adequate data for key physical-chemical, environmental fate, acute ecotoxicity, and acute mammalian toxicity properties of the Alkylate Top are available. These data are summarized below.

Physical-Chemical Properties

Boiling point and water solubility information for the Alkylate Top material is available from Huntsman LLC Material Safety Data Sheets. While the quality of these data could not be adequately assessed, the boiling point values are consistent with the expected values compared to LAB.

Environmental Fate

The ultimate biodegradability (i.e., mineralization) of the Alkylate Top and other alkylated materials was evaluated in 1980 by Monsanto using a shake flask CO_2 evolution test similar to the standard ASTM practice, which is similar to the current OECD protocol. Periodic removal and titration of a barium hydroxide solution was used to determine the CO_2 evolved. Results show a mean of 46% degradation (range 43-51%) after 35 days. This represents a moderate biodegradation rate, primarily due to the degradation of the paraffin and alkylbenzene components. It should be noted that the composition of the material tested was 29% paraffin, 44% alkylbenzenes and 24% dialkylindanes/tetralins. Due to modifications in the manufacturing process, current Alkylate Top consists of 13-36% paraffin, 48-56% linear alkylbenzenes, approximately 8% dialkylindanes/tetralins, with about 6-22% iso-LAB. Since the high percentage of the less degradable dialkylindanes/tetralins would depress the overall biodegradation rate of the mixture, it is likely that this study actually represents an under-prediction of the degradation of the current Alkylate Top. Therefore, the available data indicate that current Alkylate Top will biodegrade in the environment.

Aquatic Toxicity

The aquatic toxicity of the Alkylate Top was determined by ABC Laboratories in 1981 using a standard fish toxicity test under GLP conditions. Fathead minnows were exposed to five nominal concentrations ranging from 100 to 1000 mg/L for 96 hours. Acetone was used as a solvent to assist in dissolving the test material to levels significantly over its water solubility limit (as evidenced by an oily film on the surface of all test solutions). No mortality or sublethal effects were observed and the 96-hour LC_{50} value was determined to be greater than 1000 mg/L.

Mammalian Toxicity

The acute toxicity of the Alkylate Top mixture has been evaluated in a series of studies conducted in the early and late 1970s by Younger Laboratories. Oral toxicity studies in rats were conducted in 1973 at a limit dose of 15,800 mg/kg, and were repeated in 1978 at a limit dose of 10,000 mg/kg. In both sets of studies, rats were given a single undiluted dose of L210L or L210H (both CAS#68608-80-0) by gavage and observed for 14 days. No mortality was observed in any of the studies at these doses, resulting in oral LD_{50} values greater than 15,800 mg/kg and 10,000 mg/kg.

Acute dermal studies were conducted at the same time as the oral studies. Undiluted L210L or L210H was applied to the intact skin of New Zealand albino rabbits for 24 hours and the rabbits were observed for 14 days. Results indicate acute LD_{50} values of greater than 5,010 mg/kg in both the earlier tests and greater than 2,000 mg/kg and 1,260 mg/kg for the L210L and L210H, respectively, in the later tests. Rabbits treated with higher doses (e.g., 7,940 mg/kg in the earlier tests, 5,010 mg/kg in the later tests) experienced mortality and gross visceral alterations during the studies.

Acute inhalation studies were also conducted by Younger Laboratories. For these tests, Sprague-Dawley albino male rats were exposed to vapor concentrations of L210L or L210H ranging up to

0.9 mg/L. Rats were held in 35 L exposure chambers with the test materials for 6 hours at 27 ºC, then removed and observed for 14 days. No mortality or other toxic signs were observed in any of the tests conducted.

In summary, adequate data are available for the sponsored Alkylate Top to characterize its acute mammalian toxicity. Results show that the Alkylate Top mixture tested is not acutely toxic at environmentally relevant levels. Single dose oral and inhalation studies result in no observable acute toxicity, and the dermal exposures result in acute toxicity only at extremely high levels. It can be concluded that the Alkylate Top does not present an unreasonable acute risk to mammals.

Summary of the Available Data on the Alkylate Top

Adequate data exist to characterize the biodegradation, acute toxicity to fish, and acute toxicity to mammals of the sponsored Alkylate Top. These data demonstrate that the Alkylate Top will undergo substantial degradation in the environment and does not present an acute toxicity concern for fish or mammals. The sole use of Alkylate Top as a component that is blended into marine diesel fuel, which then undergoes destruction during the combustion process, significantly limits any exposure potential.

Specific data are not available to characterize the Alkylate Top mixture's toxicity to aquatic invertebrates or to characterize the potential effects of long-term mammalian exposure. Therefore, the available environmental fate and toxicity data for the principal constituents of the mixture have been reviewed and evaluated in order to assist in the characterization of the Alkylate Top. Data for the structurally similar primary alkylbenzenes were also evaluated when data were available. Given the mixture's production in the LAB production process, comparison to the properties of LAB is also appropriate. This evaluation is summarized below.

B. *Evaluation of the Available Data on LAB and the Constituent Compounds*

As discussed above, the principal constituents of the Alkylate Top mixture are secondary alkylbenzenes (primarily C_{10}-LAB) and paraffins (specifically, tetradecane and pentadecane).

Physical-Chemical Properties

As can be seen in Table A-1, the principal constituents and structurally related materials all have very similar and predictable physical-chemical properties. All have boiling points less than LAB, as is necessitated by the distillation process by which the Alkylate Top mixture and its constituents are produced. All of the constituents are of low to moderate volatility and very low water solubility. The reported log octanol/water partition coefficients are all very high and fall within a narrow range of 7.11 to 7.72. These data indicate similarity with the existing data for the Alkylate Top and LAB. While data on the physical-chemical properties of the Alkylate Top itself are limited, the data for the principal constituents show a consistency that allows for the estimation of properties for the sponsored mixture. Based on the sum of the information one can predict that the Alkylate Top will have a low to moderate volatility, low water solubility and high octanol/water partitioning.

Environmental Fate

Studies conducted on the Alkylate Top indicate that it biodegrades under environmental conditions. Available data for its constituents also indicate substantial biodegradation.

Aquatic Toxicity

A study conducted on the Alkylate Top demonstrates that the mixture is not acutely toxic to fish even at concentrations enhanced via solvents to levels much greater than its solubility in water. Studies conducted on decylbenzene confirm that the material is not acutely toxic to fish or *Daphnia* at the water solubility limit. Furthermore, data for LAB also demonstrate no acute toxicity to fish, *Daphnia*, or algae at saturation. Exposure to enhanced concentrations using solvents also do not result in toxicity to algae and the EC_{50} for *Daphnia* is 1.1 mg/L – far above the solubility limit of LAB. Given the structural similarities between the Alkylate Top, LAB, and the constituent materials, one would expect that toxicity to fish, *Daphnia* and algae would be similar. Thus, no acute toxicity at the water solubility limit would be expected. Chronic aquatic toxicity data are not available, but environmental exposure is limited to spill situations and therefore chronic exposures are very unlikely. In addition, the estimated log K_{ow} values of the constituents are generally high (7.11-9.12), falling at or above the range of values that would suggest the need for chronic testing.

Mammalian Toxicity

The Alkylate Top has been adequately characterized for acute toxicity, as described above, and does not present a concern. Data for all of the other endpoints are available for LAB (Table A-1) and indicate low concern. The presence of significant levels of LAB constituents (e.g., C_{10}-LAB, dialyklindanes/tetralins, iso-LABs) in Alkylate Top (Table 1) and the consistency of the acute toxicity data between LAB and Alkylate Top indicate that the Alkylate Top would be expected to show a similar lack of genotoxicity and chronic toxicity. While LAB does not contain the paraffin constituents found in the Alkylate top, the acute toxicity data for pentadecane and the repeated dose value for tetradecane support the low concern for the Alkylate Top. The lack of significant exposure potential also indicates a lack of toxicological concern for the Alkylate Top.

VI. SUMMARY OF THE AVAILABLE DATA

The sponsored Alkylate Top is a mixture of aromatic and aliphatic hydrocarbons derived as a low boiling point co-product from the LAB manufacturing process. Available data indicate that the Alkylate Top has very low solubility in water, will biodegrade in the environment, will not be acutely toxic to aquatic organisms at its water solubility limit, and is not acutely toxic to mammals by the oral or inhalation routes of exposure. No acute effects were observed at relatively high doses following dermal exposures, although some effects were noted at extremely high dermal contact with the material. However, the exclusive use of the Alkylate Top mixture as a component blended into marine diesel fuel significantly limits environmental and consumer exposure. The Alkylate Top manufacturing process is closed and workers can use personal protective equipment to effectively minimize risk. Data for LAB and *n*-paraffins, the principal

constituents of the mixture, as well as structurally related alkylbenzenes help to fill in any gaps in the characterization of the Alkylate Top.

VII. CONCLUSIONS

Given the availability of data for the key endpoints, the biodegradation potential, the lack of significant toxicity concerns, and the extremely limited exposure potential, no further testing is deemed necessary to characterize the Alkylate Top mixture.

VIII. REFERENCES

De Almeida, J.L.G., Dufax, M., Ben Taarit, Y. and Naccache, C. 1994. Linear alkyl benzene. J. Am. Chem. Soc. 71:675ff.

European Risk Assessment Report for Benzene C_{10-13} Alkyl Derivs, CAS #67774-74-7 (last revision June 1997).

Nielsen, A.M., Britton, L.N., Beall, C.E., McCormick, T.P., and Russell, G.L. 1997. Biodegradation of co-products of commercial linear alkylbenzene sulfonate. Environ. Sci. Technol. 31:3397-3404.

Rapko, J. 2002. Summary of L210 Analyses.

USEPA. 2002. Updated LAB SIDS report. (SIDS Initial Assessment Report (SIAR), Benzene, C10-16 Alkyl Derivatives, CAS Nos. 123-01-3, etc.)

Table A-1
Summary of Data Available for the LAB Alkylate Top

Section	Description	Benzene C10-13 alkyl derivs. (LAB)	Benzene, C6-12 alkyl derivatives "Alkylate Top"	Pentadecane (C15 normal paraffin)	Tetradecane (C14 normal paraffin)	C10-LAB	Decylbenzene	Nonylbenzene
	CAS Number	**67774-74-7**	**68608-80-0**	**629-62-9**	**629-59-4**	**340017-14-3**	**104-72-3**	**1081-77-2**
	Physical-Chemical Data							
2.1	Melting Point	< -70°C	--	10 C	6 C	--	-14 C	-24 C
2.2	Boiling Point	278-314°C	240-250 C	271 C	253 C	276-286 C 262-286 C **	300 C	282 C
2.4	Vapour Pressure	0.017 hPa *	--	0.0046 hPa	0.0155 hPa	--	0.0017 hPa	0.0076 hPa *
2.5	Octanol/Water Partition Coefficient (log)	7.5-9.12 *	--	7.72	7.2	7.5	7.35	7.11 *
2.6.1	Water Solubility	0.041 mg/L at 27°C 0.037 mg/L	< 1,000 mg/L	0.00008 mg/L	0.0022 mg/L	0.040 mg/L	0.0024 mg/L	0.035 mg/L *
	Environmental Fate and Pathways							
3.1.1	Photodegradation	< 1% after 14 days	--	$t_{1/2}$ = 7.1 hrs *	$t_{1/2}$ = 7.7 hrs *		$t_{1/2}$ = 7.5 hrs *	$t_{1/2}$ = 8.1 hrs *
3.1.2	Stability in Water	--	stable	--	--	--	--	--
3.5	Biodegradation	56-61% biodeg after 35 days 64-67% biodeg after 28 days	46% after 35 days	100% in seawater in 8 weeks; 75% degradation by sediment microbes in 8 days	100% in seawater in 8 weeks; Biodegrades easily	--	--	65% after 10 days; 72% degradation by sediment microbes in 8 days
	Ecotoxicity							
4.1	Acute/Prolonged Toxicity to Fish	No effects up to soluble limits LC_{50} > 1,000 mg/L with a solvent	LC_{50} >1,000 mg/L with a solvent	NOEC > 1240 ppm	NOEC > 2110 ppm	LC_{50} > Water Solubility (0.079 mg/L)	--	--
4.2	Acute Toxicity to Daphnia	No effects at saturated concentration (up to 0.041 mg/L); EC_{50} = 1.1 mg/L with a solvent	--	--	--	EC_{50} > 0.10 mg/L	--	--
4.3	Toxicity to Aquatic Plants (e.g., algae)	No effects up to soluble limits EC_{50} > 1,000 mg/L with a solvent	--	--	--	EC50 > 0.10 mg/L	--	--
	Toxicity							
5.1.1	Acute Oral Toxicity	LD_{50} (rat) > 5,000 mg/kg	LD_{50}(rat) >10,000; >15,800 mg/kg	--	--	--	--	--
5.1.2	Acute Inhalation Toxicity	LC_{50} > 1.82 mg/L LC_{50} = 71 mg/L	No toxic effects after 6 hours at concentrations of up to 0.9 mg/L	--	--	--	--	--
5.1.3	Acute Dermal Toxicity	LD_{50} > 2,000 mg/kg	LD_{50}(rabbit) >2000; >1,260; >5,010 mg/kg	--	--	--	--	--
5.1.4	Acute Toxicity by Other Routes	--	--	LD_{50}(i.v., mouse) = 3493 mg/kg	--	--	--	--
5.4	Repeated Dose Toxicity	NOEL = 102 mg/m^3 (inhalation) LOEL = 125 mg/kg (oral)	--	--	TD_{LO}(mice) = 9600 mg/kg for 20 weeks		--	--
5.5	Genetic Toxicity in-vitro (Bacterial test)	Negative	--	--	--	--	--	--
5.5	Genetic Toxicity in-vitro (Non-bacterial test)	Negative	--	--	--	--	--	--
5.6	Genetic Toxicity in-vivo	Negative	--	--	--	--	--	--
5.8	Toxicity to Reproduction	NOAEL (maternal) = 50 mg/kg NOAEL (fetal) = 50 mg/kg	--	--	--	--	--	--
5.9	Developmental Toxicity/Teratogenicity	NOAEL (maternal) = 125 mg/kg Not teratogenic	--	--	--	--	--	--

* Estimated Values
** Estimated data for C9-LAB based on regression analysis